



TITLE:

2. DNA二重らせんと水和水 : 低振動  
数ラマン散乱(お茶の水女子大学理  
学研究科物理学専攻, 修士論文題目  
・ アブストラクト(1986年度), その  
2)

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CITATION:

小川, 恵. 2. DNA二重らせんと水和水 : 低振動数ラマン散乱(お茶の水女子大学理学研究科物理学専攻, 修士論文題目・アブストラクト(1986年度), その2). 物性研究 1987, 48(5): 563-566

ISSUE DATE:

1987-08-20

URL:

<http://hdl.handle.net/2433/92780>

RIGHT:

theory, an expansion formula is obtained for the current-current correlation function. The conductivity tensor is calculated as the Fourier-Laplace transform of the current-current correlation function to give the absorption spectrum.

The absorption spectra are numerically calculated for two- and three-dimensional electron systems within the second order approximation of the impurity potential. The relating potential is assumed to be Gaussian. Since in existing works numerical calculations for the explicit form of absorption spectrum have been performed so rarely, our calculations are considered to be important.

Our method has a quite satisfactory feature : a direct calculation of the correlation function can be performed without the use of the regression theorem. Furthermore owing to this method the average over random configurations of the impurities can be performed rigorously. In this thesis our consideration is restricted to the second order of the perturbation. However it may be possible to renormalize higher order terms with a resummation technique like CPA, since higher order terms can be calculated systematically.

## 2. DNA二重らせんと水和水 —低振動数ラマン散乱—

小 川 恵

### Abstract

Recently it has been of great interest to study the dynamical properties of the molecular assembly of DNA double helix in connection with the hydrated water, because the hydrated water around DNA affects strongly not only the local conformation of the double helix but also the

global association of the molecular assembly. Although numerous investigations on DNA have been carried out in the dilute solution, there has been only few investigation in the condensed state. The effect of the hydrated water to the dynamical structure of DNA double helix plays an important role on biological function and it appears more drastically in the condensed state than in the dilute solution.

The purpose of the present work is to clarify the dynamical properties of the hydrated water of the condensed DNA by means of the low frequency Raman spectroscopy. During the melting process of DNA double helix in the condensed state, it is expected that the relaxation time of the hydrated water (the primary hydration shell) changes by order of magnitude. In this case the low frequency Raman spectra can be strongly affected not only by the collective vibration of the double helix but also by the relaxational motion of the hydrated water.

In condensed DNA double helix there exist two kinds of collective vibrational modes in the low frequency Raman spectral region. One is the broad band ( $30\sim 100\text{cm}^{-1}$ ) which gradually turns into the central component during the melting process of the double helix both in the dilute solution and in the condensed state. The other is the sharp mode (S-mode) at  $\sim 16\text{cm}^{-1}$  in B-DNA fiber and at  $\sim 22\text{cm}^{-1}$  in A-DNA solid at room temperature. This S-mode exists only in the condensed state and disappears when the periodic arrangement of the double helix vanishes.

Samples used here are Calf-thymus DNA from Miles cooperation. Three kinds of specimen were prepared in order to reveal the dynamics of the hydrated water. One is the B-DNA gel which includes both the primary hydration shell and the secondary hydration shell, the second is the A-DNA solid which includes only the primary hydration shell, and the third is the dry-DNA which includes no hydrated water. The temperature dependence ( $-140^\circ\text{C}\sim 120^\circ\text{C}$ ) of the low frequency Raman spectra ( $\leq 50\text{cm}^{-1}$  or  $\leq 200\text{cm}^{-1}$ ) was obtained as well as the high frequency Raman spectra

( $700\text{cm}^{-1}$  ~  $950\text{cm}^{-1}$ ) which show the local conformation of the DNA molecule.

The coupled mode analysis has been carried out on the S-mode spectra between the collective vibrational mode of the DNA double helix and the relaxational mode of the hydrated water. The following results have been obtained.

(1) In the B-DNA gel the relaxation time of the secondary hydration shell  $\tau_2$  drastically decreases (becomes fast) with increasing temperature around  $-20^\circ\text{C}$ . This causes the drastic change of the S-mode spectra from the oscillatory type to the relaxational type. The relaxation time of the primary hydration shell  $\tau_1$  monotonically decreases with increasing temperature from  $-40^\circ\text{C}$  to  $100^\circ\text{C}$  where the double helix is melted out. It is noticed that the value of  $\tau_1$  at  $100^\circ\text{C}$  is  $\sim 6 \times 10^{-12}\text{s}$  which is the same value of the relaxation time of the bulk water at  $0^\circ\text{C}$ .

(2) In the A-DNA solid the relaxation time of the primary hydration shell  $\tau_1$  monotonically decreases with increasing temperature from  $-40^\circ\text{C}$  to  $100^\circ\text{C}$  where the double helix is melted out. This temperature dependence of  $\tau_1$  is very similar to that of the B-DNA gel. It is worth noting that although the spectral feature of the S-mode is completely different between the B-DNA gel and the A-DNA solid, the relaxation time of the primary hydration shell obeys similar temperature dependence up to the melting temperature.

(3) In the dry-DNA, the melting of the double helix has never occurred until  $120^\circ\text{C}$ . Neither the low frequency spectra nor the high frequency spectra change in whole temperature region ( $-140^\circ\text{C}$  ~  $120^\circ\text{C}$ ). This means that the

existence of the hydrated water, especially the primary hydration shell, is indispensable to the melting of the double helix.

(4) It has been reconfirmed that the S-mode appears only when the periodic arrangements of the double helix exist. In connection with this result it has been found that in the dry-DNA there exists no S-mode. The low frequency response at  $\sim 30\text{cm}^{-1}$  is assigned to the broad band.

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|--|---------|
| 1. 高速電子衝突実験装置                              | 福 島 聡   |
| 2. 圧電素子のパルス駆動方式                            | 杉 山 茂 孝 |
| 3. GaAs からの光電子                             | 隅 田 佳 文 |
| 4. Zn 原子の低エネルギー電子衝撃による励起・発光                | 高 井 潔   |
| 5. 核研ニュートリノ質量測定実験における原子・分子効果               | 滝 沢 誠   |
| 6. SU(3) Cloudy Bag Model による 8 重項重粒子の磁気能率 | 山 口 哲 哉 |
| 7. Ne の KLL オージェ電子の PCI 効果                 | 山 口 寿 男 |

### 1. 高速電子衝突実験装置

福 島 聡

高速電子の原子・分子による非弾性小角散乱は、光吸収または光イオン化過程のシミュレーションとして応用できる。我々の研究室では、シンクロトロン軌道放射光波長域での光吸収、光イオン化及び光電子分光と同等の実験をエネルギー損失分光法を用いた高速電子の散乱実験により、実現し、また原子・分子の内殻励起、電離過程の研究を行うことを目的とした新しい実験装置を製作した。

光学的振動子強度  $f_{\text{opt}}$  と一般化振動子強度  $F(k)$  の間には